

(2E)-1-(4-Bromophenyl)-3-[4-(methylsulfanyl)phenyl]prop-2-en-1-oneRay J. Butcher,^a Jerry P. Jasinski,^{b*} H. S. Yathirajan,^c
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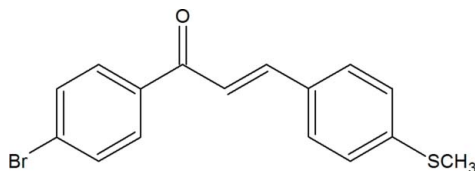
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}—\text{C}) = 0.006$ Å; R factor = 0.035; wR factor = 0.078; data-to-parameter ratio = 12.1.

In the title molecule, $\text{C}_{16}\text{H}_{13}\text{BrOS}$, the mean planes of the 4-bromophenyl and 4-(methylsulfanyl)phenyl groups are twisted by $47.4(2)^\circ$ from each other. The angles between the mean plane of the prop-2-en-1-one group and those of the 4-bromophenyl and 4-(methylsulfanyl)phenyl groups are $21.1(4)$ and $26.3(2)^\circ$, respectively. Crystal packing is characterized by alignment of adjacent molecules *syn* to each other, oblique to the *ac* plane and stacked in parallel arrays along the *c* axis of the unit cell. The closest distance between 4-bromophenyl rings is $4.536(2)$ Å; that between 4-(methylsulfanyl)phenyl groups is $4.539(2)$ Å.

Related literature

For related structures, see: Butcher, Yathirajan, Sarojini *et al.* (2006); Butcher, Yathirajan, Anilkumar *et al.* 2006*a,b,c*. For related background, see: Dimmock *et al.* (1999); Lawrence *et al.* (2001); Phrutivorapongkul *et al.* (2003); Xia *et al.* (2000); Pandey *et al.* (2005); Uchida *et al.* (1998); Goto *et al.* (1991); Tam *et al.* (1989); Indira *et al.* (2002); Fichou *et al.* (1988) and Cho *et al.* (1996).

**Experimental***Crystal data* $\text{C}_{16}\text{H}_{13}\text{BrOS}$
 $M_r = 333.23$ Monoclinic, Cc
 $a = 33.729(6)$ Å $b = 6.9503(12)$ Å
 $c = 5.8487(10)$ Å
 $\beta = 90.868(3)^\circ$
 $V = 1371.0(4)$ Å³
 $Z = 4$ Mo $K\alpha$ radiation
 $\mu = 3.14 \text{ mm}^{-1}$
 $T = 100$ K
 $0.60 \times 0.50 \times 0.39$ mm*Data collection*Bruker APEXII CCD
diffractometer
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.515$, $T_{\max} = 1.000$
(expected range = 0.151–0.294)7498 measured reflections
2086 independent reflections
1986 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.049$ *Refinement* $R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.078$
 $S = 1.53$
2086 reflections
173 parameters
2 restraintsH-atom parameters constrained
 $\Delta\rho_{\max} = 1.05 \text{ e Å}^{-3}$
 $\Delta\rho_{\min} = -0.45 \text{ e Å}^{-3}$
Absolute structure: Flack (1983),
with 1949 Friedel pairs
Flack parameter: 0.016 (5)

Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Bruker, 2000).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2019).

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supplementary materials

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(2E)-1-(4-Bromophenyl)-3-[4-(methylsulfanyl)phenyl]prop-2-en-1-one

R. J. Butcher, J. P. Jasinski, H. S. Yathirajan, B. Narayana and A. Mithun

Comment

Chalcones possess a broad spectrum of biological activities, including antibacterial, antihelmintic, amoebicidal, anti-ulcer, antiviral, insecticidal, antiprotozoal, anticancer, cytotoxic and immunosuppressive activities. Among the various organic compounds reported for their non-linear optical (NLO) properties, chalcone derivatives are notable for their excellent blue-light transmittance and good crystallizability. They provide a necessary molecular electronic configuration to show NLO effects, with two aromatic rings connected through a conjugated bridge. Substitution on either of the benzene rings appears to increase the likelihood of non-centrosymmetric crystal packing, as well as enhancing the electronic properties of the molecule. The molecular hyperpolarizability β are strongly influenced not only by the electronic effect but also by the steric effect of the substituent. In continuation of our quest to discover newer materials, we have synthesized a new chalcone derivative and studied its SHG efficiency. The SHG efficiency of the title compound is found to be five times that of urea. In view of the importance of the title compound, (I), $C_{16}H_{13}BrOS$, a crystal structure is reported here.

The mean planes of the 4-bromophenyl and 4-(methylsulfanyl)phenyl groups are coplanar and twisted by $47.4(2)^\circ$ from each other (Fig. 1). The angles between the mean plane of the prop-2-en-1-one group and that of the 4-bromophenyl [torsion angle (C8–C7–C1–C2) = $159.15(18)^\circ$] and 4-(methylsulfanyl)phenyl [torsion angle (C8–C9–C10–C15) = $178.5(2)^\circ$] groups are $21.1(4)^\circ$ and $26.3(2)^\circ$, respectively.

Crystal packing is highlighted by alignment of adjacent molecules *syn* to each other, oblique to the *ac* plane and stacked in parallel arrays along the *c* axis of the unit cell. The closest distance between mean planes of the coplanar 4-bromophenyl and 4-(methylsulfanyl)phenyl groups is $4.536(2)$ and $4.539(2)$ Å, respectively (Fig. 2).

Experimental

To a mixture of 4-methylsulfanylbenzaldehyde (1.52 g, 0.01 mol) and 4-bromo-acetophenone (1.99 g, 0.01 mol) in ethanol (25 ml), a solution of potassium hydroxide (5%, 5 ml) was added slowly with stirring (Fig. 3). The mixture was stirred at room temperature for 24 h. The precipitated solid was filtered, washed with water, dried and recrystallized from acetone- toluene mixture (9:1), with a yield of 85% (m.p.: 430 K). Analysis found: C 57.55, H 3.72%; $C_{16}H_{13}BrOS$ requires: C 57.67, H 3.93%.

Refinement

The H atoms were included in the riding model approximation with C—H = $0.95\text{--}0.98$ Å, and with $U_{iso}(H) = 1.17\text{--}1.50U_{eq}(C)$.

Figures

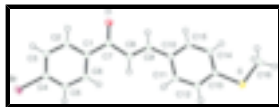


Fig. 1. Molecular structure for $C_{16}H_{13}BrOS$, (I), showing atom labeling and 50% probability displacement ellipsoids.

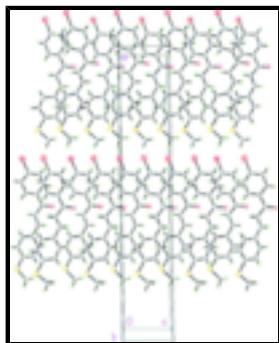


Fig. 2. Packing diagram of $C_{16}H_{13}ClBrOS$ viewed down the b axis.

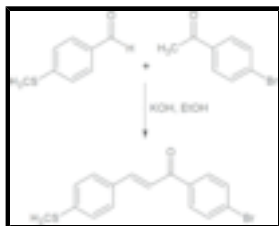


Fig. 3. The formation of the title compound, $C_{16}H_{13}BrOS$.

(2E)-1-(4-Bromophenyl)-3-[4-(methylsulfanyl)phenyl]prop-2-en-1-one

Crystal data

$C_{16}H_{13}BrOS$

$M_r = 333.23$

Monoclinic, Cc

$a = 33.729$ (6) Å

$b = 6.9503$ (12) Å

$c = 5.8487$ (10) Å

$\beta = 90.868$ (3)°

$V = 1371.0$ (4) Å³

$Z = 4$

$F_{000} = 672$

$D_x = 1.614$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 7711 reflections

$\theta = 2.4$ – 30.7°

$\mu = 3.14$ mm⁻¹

$T = 100$ K

Block, colourless

$0.60 \times 0.50 \times 0.39$ mm

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 100$ K

ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)

2086 independent reflections

1986 reflections with $I > 2\sigma(I)$

$R_{int} = 0.049$

$\theta_{max} = 30.6^\circ$

$\theta_{min} = 2.4^\circ$

$h = -48 \rightarrow 47$

$T_{\min} = 0.515$, $T_{\max} = 1.000$
7498 measured reflections

$k = -9 \rightarrow 9$
 $l = -8 \rightarrow 8$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.078$

$S = 1.53$

2086 reflections

173 parameters

2 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2)]$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 1.05 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.45 \text{ e } \text{\AA}^{-3}$

Extinction correction: none

Absolute structure: Flack (1983), with 1949 anomalous pairs

Flack parameter: 0.016 (5)

Special details

Experimental. ^1H NMR (CD_2Cl_2) δ 7.88 (d, 2H), 7.77 (d, 1H), 7.64 (d, 2H), 7.55 (d, 1H), 7.42 (d, 1H), 7.26 (d, 2H), 2.52 (s, 3H).

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br	1.120444 (16)	0.21264 (5)	0.47652 (4)	0.02440 (11)
S	0.72237 (3)	0.30093 (13)	0.31258 (15)	0.0207 (2)
O	0.94871 (10)	0.2763 (4)	1.0726 (5)	0.0253 (6)
C1	0.99256 (13)	0.2650 (5)	0.7622 (7)	0.0181 (7)
C2	1.02506 (12)	0.3265 (5)	0.8931 (7)	0.0182 (7)
H2A	1.0209	0.3782	1.0411	0.022*
C3	1.06277 (13)	0.3137 (5)	0.8122 (7)	0.0193 (7)
H3A	1.0847	0.3587	0.9011	0.023*
C4	1.06860 (13)	0.2320 (5)	0.5932 (7)	0.0197 (7)
C5	1.03697 (12)	0.1710 (5)	0.4606 (7)	0.0187 (7)
H5A	1.0412	0.1172	0.3136	0.022*
C6	0.99861 (12)	0.1887 (5)	0.5438 (7)	0.0182 (7)
H6A	0.9766	0.1491	0.4523	0.022*

supplementary materials

C7	0.95225 (14)	0.2734 (5)	0.8619 (7)	0.0200 (7)
C8	0.91725 (15)	0.2746 (5)	0.7062 (7)	0.0188 (7)
H8A	0.9199	0.3109	0.5506	0.023*
C9	0.88213 (15)	0.2243 (5)	0.7859 (7)	0.0177 (7)
H9A	0.8817	0.1783	0.9388	0.021*
C10	0.84376 (14)	0.2322 (5)	0.6626 (7)	0.0160 (7)
C11	0.83901 (11)	0.3127 (5)	0.4409 (6)	0.0169 (7)
H11A	0.8617	0.3544	0.3605	0.020*
C12	0.80217 (12)	0.3315 (5)	0.3408 (6)	0.0171 (7)
H12A	0.7996	0.3870	0.1928	0.020*
C13	0.76798 (12)	0.2691 (5)	0.4555 (6)	0.0166 (7)
C14	0.77203 (12)	0.1864 (5)	0.6720 (7)	0.0173 (7)
H14A	0.7494	0.1419	0.7506	0.021*
C15	0.80961 (12)	0.1698 (5)	0.7717 (6)	0.0158 (7)
H15A	0.8121	0.1139	0.9195	0.019*
C16	0.68734 (13)	0.2242 (6)	0.5225 (8)	0.0285 (9)
H16A	0.6603	0.2445	0.4633	0.043*
H16B	0.6913	0.2990	0.6630	0.043*
H16C	0.6913	0.0873	0.5555	0.043*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.01786 (18)	0.03035 (19)	0.02513 (18)	0.0017 (2)	0.00495 (13)	−0.0012 (2)
S	0.0181 (5)	0.0240 (5)	0.0198 (4)	0.0002 (3)	−0.0026 (4)	0.0017 (4)
O	0.0216 (16)	0.0394 (18)	0.0150 (13)	0.0021 (13)	−0.0020 (12)	0.0013 (12)
C1	0.0207 (19)	0.0169 (16)	0.0167 (16)	0.0017 (13)	0.0015 (14)	0.0028 (13)
C2	0.0232 (19)	0.0111 (14)	0.0203 (16)	0.0024 (12)	−0.0008 (14)	−0.0009 (13)
C3	0.0199 (17)	0.0184 (17)	0.0194 (18)	−0.0007 (13)	−0.0033 (14)	0.0002 (13)
C4	0.0225 (19)	0.0168 (16)	0.0200 (17)	0.0019 (13)	0.0023 (14)	0.0025 (13)
C5	0.023 (2)	0.0164 (16)	0.0172 (17)	0.0024 (13)	0.0023 (15)	0.0000 (13)
C6	0.0201 (18)	0.0152 (16)	0.0193 (16)	0.0007 (12)	−0.0037 (14)	0.0010 (13)
C7	0.022 (2)	0.0162 (16)	0.0213 (18)	0.0031 (14)	−0.0021 (16)	−0.0008 (14)
C8	0.019 (2)	0.0206 (19)	0.0172 (17)	−0.0005 (14)	−0.0021 (16)	−0.0015 (14)
C9	0.023 (2)	0.0154 (17)	0.0144 (16)	−0.0014 (14)	0.0000 (15)	−0.0011 (13)
C10	0.019 (2)	0.0135 (16)	0.0152 (17)	−0.0028 (13)	0.0016 (16)	0.0000 (13)
C11	0.0184 (17)	0.0162 (16)	0.0161 (16)	−0.0003 (11)	0.0032 (14)	0.0000 (12)
C12	0.0224 (19)	0.0142 (14)	0.0147 (17)	−0.0013 (14)	0.0020 (14)	0.0001 (13)
C13	0.0182 (18)	0.0173 (16)	0.0143 (15)	−0.0001 (12)	−0.0001 (14)	−0.0003 (12)
C14	0.0177 (19)	0.0172 (16)	0.0170 (16)	−0.0024 (13)	0.0036 (14)	−0.0019 (13)
C15	0.0177 (19)	0.0157 (15)	0.0139 (16)	0.0004 (13)	0.0007 (14)	−0.0013 (13)
C16	0.016 (2)	0.040 (2)	0.029 (2)	−0.0035 (16)	0.0028 (17)	0.0044 (18)

Geometric parameters (\AA , $^\circ$)

Br—C4	1.892 (4)	C8—H8A	0.9500
S—C13	1.754 (4)	C9—C10	1.473 (7)
S—C16	1.798 (5)	C9—H9A	0.9500
O—C7	1.240 (5)	C10—C15	1.395 (6)

C1—C2	1.394 (6)	C10—C11	1.419 (5)
C1—C6	1.401 (5)	C11—C12	1.372 (6)
C1—C7	1.489 (6)	C11—H11A	0.9500
C2—C3	1.367 (6)	C12—C13	1.411 (5)
C2—H2A	0.9500	C12—H12A	0.9500
C3—C4	1.417 (5)	C13—C14	1.395 (5)
C3—H3A	0.9500	C14—C15	1.392 (6)
C4—C5	1.377 (6)	C14—H14A	0.9500
C5—C6	1.394 (6)	C15—H15A	0.9500
C5—H5A	0.9500	C16—H16A	0.9800
C6—H6A	0.9500	C16—H16B	0.9800
C7—C8	1.480 (6)	C16—H16C	0.9800
C8—C9	1.326 (6)		
C13—S—C16	102.6 (2)	C8—C9—H9A	116.5
C2—C1—C6	119.5 (4)	C10—C9—H9A	116.5
C2—C1—C7	119.2 (3)	C15—C10—C11	117.3 (4)
C6—C1—C7	121.2 (4)	C15—C10—C9	119.3 (3)
C3—C2—C1	121.2 (3)	C11—C10—C9	123.2 (4)
C3—C2—H2A	119.4	C12—C11—C10	121.1 (4)
C1—C2—H2A	119.4	C12—C11—H11A	119.4
C2—C3—C4	118.8 (4)	C10—C11—H11A	119.4
C2—C3—H3A	120.6	C11—C12—C13	120.6 (4)
C4—C3—H3A	120.6	C11—C12—H12A	119.7
C5—C4—C3	121.0 (4)	C13—C12—H12A	119.7
C5—C4—Br	119.2 (3)	C14—C13—C12	119.3 (4)
C3—C4—Br	119.7 (3)	C14—C13—S	123.9 (3)
C4—C5—C6	119.4 (4)	C12—C13—S	116.9 (3)
C4—C5—H5A	120.3	C15—C14—C13	119.4 (4)
C6—C5—H5A	120.3	C15—C14—H14A	120.3
C5—C6—C1	120.0 (4)	C13—C14—H14A	120.3
C5—C6—H6A	120.0	C14—C15—C10	122.4 (4)
C1—C6—H6A	120.0	C14—C15—H15A	118.8
O—C7—C8	121.6 (4)	C10—C15—H15A	118.8
O—C7—C1	119.5 (4)	S—C16—H16A	109.5
C8—C7—C1	118.9 (4)	S—C16—H16B	109.5
C9—C8—C7	119.4 (4)	H16A—C16—H16B	109.5
C9—C8—H8A	120.3	S—C16—H16C	109.5
C7—C8—H8A	120.3	H16A—C16—H16C	109.5
C8—C9—C10	126.9 (4)	H16B—C16—H16C	109.5
C6—C1—C2—C3	0.0 (5)	C7—C8—C9—C10	174.5 (3)
C7—C1—C2—C3	177.2 (3)	C8—C9—C10—C15	178.7 (4)
C1—C2—C3—C4	−1.5 (5)	C8—C9—C10—C11	−5.6 (6)
C2—C3—C4—C5	1.7 (5)	C15—C10—C11—C12	1.2 (5)
C2—C3—C4—Br	179.9 (3)	C9—C10—C11—C12	−174.5 (3)
C3—C4—C5—C6	−0.4 (5)	C10—C11—C12—C13	−0.6 (5)
Br—C4—C5—C6	−178.6 (3)	C11—C12—C13—C14	−0.5 (5)
C4—C5—C6—C1	−1.1 (5)	C11—C12—C13—S	179.7 (3)
C2—C1—C6—C5	1.4 (5)	C16—S—C13—C14	4.9 (4)

supplementary materials

C7—C1—C6—C5	−175.8 (3)	C16—S—C13—C12	−175.2 (3)
C2—C1—C7—O	−22.1 (5)	C12—C13—C14—C15	0.9 (5)
C6—C1—C7—O	155.0 (4)	S—C13—C14—C15	−179.2 (3)
C2—C1—C7—C8	159.0 (3)	C13—C14—C15—C10	−0.3 (5)
C6—C1—C7—C8	−23.9 (5)	C11—C10—C15—C14	−0.8 (5)
O—C7—C8—C9	−19.0 (6)	C9—C10—C15—C14	175.1 (3)
C1—C7—C8—C9	159.8 (3)		

Fig. 1

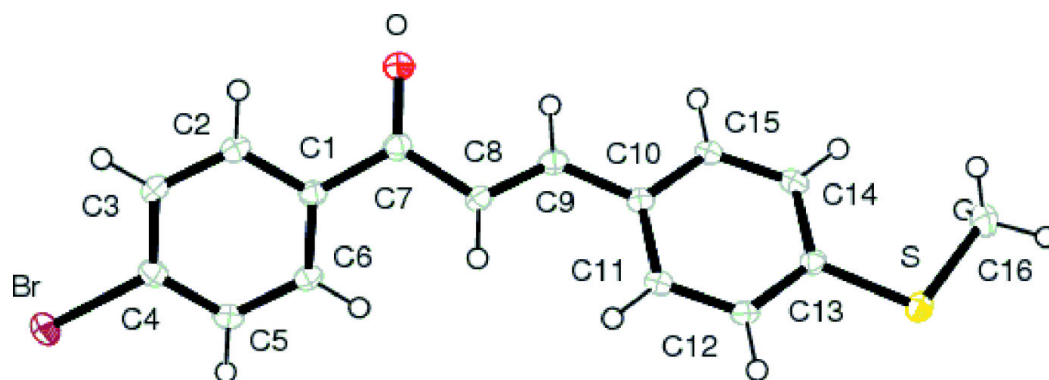


Fig. 2

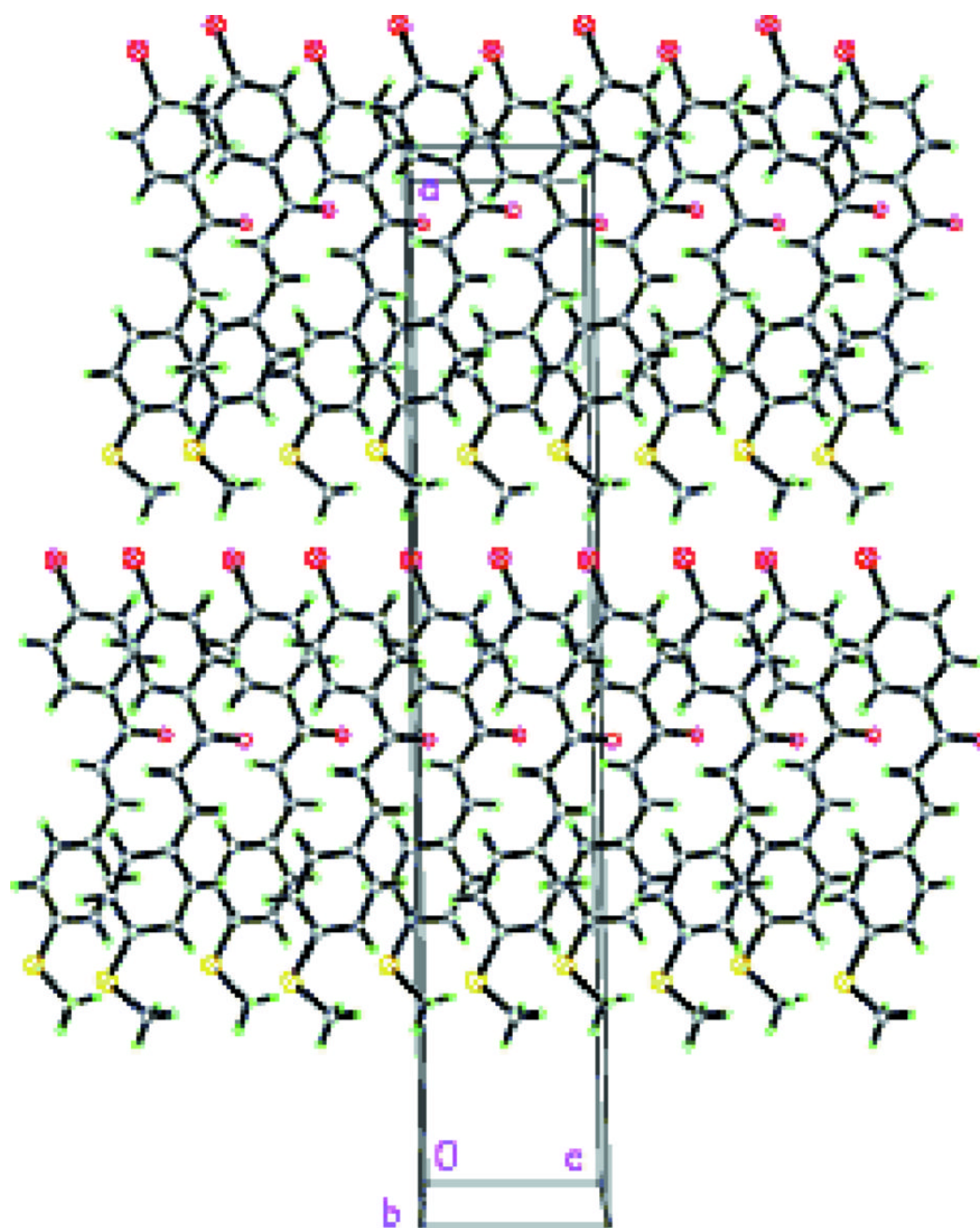


Fig. 3

